ABSTRACT

--In complex separations, more than one entity may have the same molecular weight, to within the ability of an instrument to distinguish. Accurate mass measurements are used in light of the previously unknown regularities in retention time to determine a retention time (N pairs of values $(t_i^B, t_i^{B_{ref}})$) (506). The retention time map allows a reference retention time to be assigned to each entity in a separation. The reference retention times, together with accurate mass measurements, can then be used to track and to compare entities (704,708) between separations.--